

Message

**From:** Cleston Lange [clange@mmm.com]  
**Sent:** 10/11/2017 5:51:48 PM  
**To:** Libelo, Laurence [Libelo.Laurence@epa.gov]  
**Subject:** RE: pchem data for PFHxA

Hi Laurence,

To the best of my knowledge most phys/chem info for PFHxS, and many PFAS in general, are based on in silico prediction programs, some of which don't predict well. I believe COSMOtherm is probably the most accurate and closest to achieving near the known values for PFAS when experimental values have been available. Interestingly, I was just looking at these publications myself this morning, so have these references handy. Also, the concawe report no 8/16 "Environmental fate and effects of poly and perfluoroalkyl substances (PFAS)" has a couple of nice summary tables on what is known or is predicted on PFAS. I have copied the references and links below.

Wang, Z. Macleod M. Cousings I.t. Scheringer M and Hungerbuhler K. 2011. "Using COSMOtherm to predict physicochemical properties of poly- and perfluorinated alkyl substances (PFASs)" *Environ. Chem.* 2011, 8, 389–398. [http://www.publish.csiro.au/EN/acc/EN10143/EN10143\\_AC.pdf](http://www.publish.csiro.au/EN/acc/EN10143/EN10143_AC.pdf)

Gomis, M. I., Wang Z. , M. Scheringer and Cousins I.T.. 2015. *Science of the Total Environment* 505 (2015) 981–991. <https://doi.org/10.1016/j.scitotenv.2014.10.062>

[https://www.concawe.eu/wp-content/uploads/2016/06/Rpt\\_16-8.pdf](https://www.concawe.eu/wp-content/uploads/2016/06/Rpt_16-8.pdf)

Hope this helps.

Cleston



**Cleston C. Lange, Ph.D.** | Senior Specialist  
**3M Environment, Health, and Safety. EHS Laboratory**  
3M Center, 260-5N-17 | St. Paul, MN 55144-1000 | United States  
Office: +1 651-733-9860 | Mobile: Ex. 6 - Personal Privacy  
[clange@mmm.com](mailto:clange@mmm.com)



[3M.com](http://3M.com)

CONFIDENTIAL This communication is intended only for the addressee(s) named above. It contains confidential information. Unauthorized use, disclosure, dissemination or copying of this communication, or any part thereof, is strictly prohibited. If the reader of this message is not the intended recipient please notify us immediately by telephone or electronic mail and delete or destroy this message and all copies thereof, including attachments.

---

**From:** Libelo, Laurence [mailto:Libelo.Laurence@epa.gov]  
**Sent:** Wednesday, October 11, 2017 11:28 AM  
**To:** Cleston Lange <clange@mmm.com>  
**Subject:** [EXTERNAL] pchem data for PFHxA

Hi Cleston,

I am looking for p-chem and partitioning data for PFHxS but can't seem to find measured values. Do you know of a decent reference for V.P. Kow, Koa etc? Any suggestions would be greatly appreciated.

Thanks.

Laurence

3M Note: This message is from an [EXTERNAL] sender.

If you suspect this message is malicious or spam, please click on the "Report Phishing - PhishMe" icon within the Outlook Ribbon to report it for evaluation, and do NOT open any attachments or click on any links. If you are using OWA, a handheld device, or do not see the icon, please follow the instructions below:

Click [here](#) to report this email as spam